Contents

Thematic Issue on Biomolecular Simulations Editors: B. Montgomery Pettitt and Jeremy C. Smith

Forword	х
Preface	xi
Contents	xii
Pearlman, D.A., D.A. Case, J.W. Caldwell, W.S. Ross, T.E. Cheatham III, S. DeBolt, D. Ferguson, G. Seibel and P. Kollman AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules	
Berendsen, H.J.C., D. van der Spoel and R. van Drunen GROMACS: A message-passing parallel molecular dynamics implementation	43
Madura, J.D., J.M. Briggs, R.C. Wade, M.E. Davis, B.A. Luty, A. Ilin, J. Antosiewicz, M. K. Gilson, B. Bagheri, L.R. Scott and J.A. McCammon Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program	57
Lemon, A.P., P. Dauber-Osguthorpe and D.J. Osguthorpe FOCUS: a molecular dynamics analysis program. New features for the characterisation of lipid bilayers and solvated systems	97
Nelson, M., W. Humphrey, R. Kufrin, A. Gursoy, A. Dalke, L. Kale, R. Skeel and K. Schulten MDScope-a visual computing environment for structural biology	111
Lavery, R., K. Zakrzewska and H. Sklenar JUMNA (Junction minimisation of nucleic acids)	135
Elber, R., A. Roitberg, C. Simmerling, R. Goldstein, H. Li, G. Verkhivker, C. Keasar, J. Zhang and A. Ulitsky	
MOIL: A program for simulations of macromolecules	159
Kneller, G.R., V. Keiner, M. Kneller and M. Schiller nMOLDYN: A program package for a neutron scattering oriented analysis of Molecular Dynamics simulations	191
Levitt, M., M. Hirshberg, R. Sharon and V. Daggett Potential energy function and parameters for simulations of the molecular dynamics of proteins and nucleic acids in solution	215
Wako, H., S. Endo, K. Nagayama and N. Gō FEDER/2: program for static and dynamic conformational energy analysis of macro-molecules in dihedral angle space	233

Van Belle, D. and S.J. Wodak Extended Lagrangian formalism applied to temperature control and electronic polarization effects in molecular dynamics simulations	253
Guilbert, C., D. Perahia and L. Mouawad A method to explore transition paths in macromolecules. Applications to hemoglobin and phosphoglycerate kinase	263
Roux, B. The calculation of the potential of mean force using computer simulations	275
Chow, KH. and D.M. Ferguson Isothermal-isobaric molecular dynamics simulations with Monte Carlo volume sampling	283
Simonson, T. and D. Perahia Dielectric properties of proteins from simulations: tools and techniques	291
van Gunsteren, W.F., P.H. Hünenberger, A.E. Mark, P.E. Smith and I.G. Tironi Computer simulation of protein motion	305
Goodfellow, J.M., W.R. Pitt, O.S. Smart and M.A. Williams New methods for the analysis of the protein-solvent interface	321
Micu, A.M. and J.C. Smith SERENA: a program for calculating X-ray diffuse scattering intensities from molecular dynamics trajectories	331
Smith, P.E. and B.M. Pettitt Efficient Ewald electrostatic calculations for large systems	339
Author index	345